Carbon Ad-Dimer Defects in Carbon Nanotubes: A New Route to Patterned Nanotubes for Energy Applications

Scientific Achievement

A new class of patterned carbon nanotube (CNT) structures has been discovered that provides an unparalleled opportunity for engineering their electronic properties. Using density functional computations, we have found that a rich range of defect structures and electronic structure modifications are possible by the reaction of carbon dimers with CNTs. Two novel features predicted by the computer simulations make the carbon dimer defects very attractive. First, the barriers for formation of the defects are relatively low, which means that carbon dimer insertion into the CNT surface is therefore likely to be realized using established experimental techniques. Second, the electronic states introduced by the defects depend on the size and type of the CNT. As a result of these two features of carbon ad-dimers, it is possible by their controlled multiple addition to create a new class of patterned carbon nanotubes having new electronic peaks near the Fermi level.

Significance

Success in synthesis of the patterned nanotubes based on the carbon dimer reaction as predicted in this work would provide an unparalleled opportunity for creating entirely new device functionalities for a range of energy technology applications. The results open the way for computer simulations to guide synthesis of these new materials using techniques developed for the growth of ultrananocrystalline diamond. A wide window for the manipulation of peaks in the density of states in close proximity to the Fermi level is possible in the patterned CNTs. Low dimensional materials having densities of states similar to those predicted for the patterned nanotubes often display substantially improved thermoelectric performance and could provide efficient means for solar energy conversion.

Carbon Ad-Dimer Defects in Carbon Nanotubes, Physical Review Letters, in press (2006).

Performers:

M. Sternberg, L. A. Curtiss, D. M. Gruen, G. Kedziora, D. A. Horner, P. Redfern, P. Zapol

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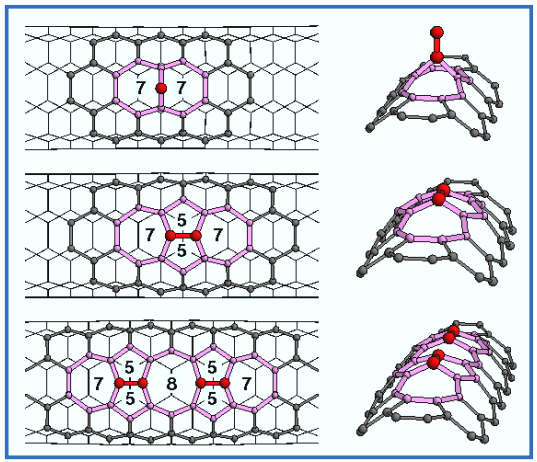

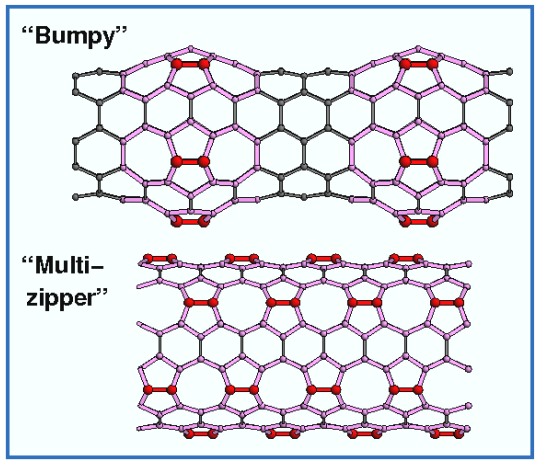

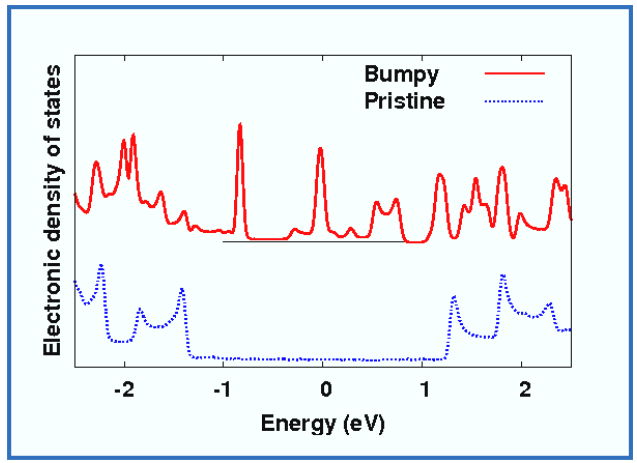

- Stages for initial C_2 adsorptions, resulting in topological defects.
- Patterned tube results from multiple controlled C_2 deposition.
- Electronic densities of states for a patterned tube. New peaks emerge near Fermi level.

- Computer simulations predict stable structures of patterned nanotubes.
- Carbon dimers can be used to modify the electronic structure of nanotubes.
- Opportunity for applications in electronic and thermoelectric devices.

M. Sternberg, L. Curtiss, D. Gruen, P. Redfern, and P. Zapol

Materials Science Division
ARGONNE NATIONAL LABORATORY

G. Kedziora (Wright Patterson AFB), D. Horner (North Central College)